

Local invariants for mixed qubit-qutrit states

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Abstract

In the present paper few steps are undertaken towards the description of the “*qubit-qutrit*” pair – quantum bipartite system composed of two and three level subsystems. The computational difficulties with the construction of the “*local unitary polynomial invariants*” are discussed. Calculations of the Molien functions and Poincaré series for the qubit-qubit and qubit-qutrit local unitary invariants are outlined and compared with the known results. The requirement of positive semi-definiteness of the density operator is formulated explicitly as a set of inequalities in five Casimir invariants of the algebra $\mathfrak{su}(6)$.

Key words: entanglement, polynomial invariants, Molien function, positive definiteness

1 Introduction

The present article discusses several computational aspects of a pure quantum effects in composite systems playing an important role in the modern theory of quantum computing and quantum information [1, 2].

The cornerstone of these latest trends is an extraordinary quantum phenomenon – the “*entanglement*” of quantum states. Basically, under the entanglement it is assumed an exposition of diverse non-local correlations in a composite multipartite quantum system, which have no classical analogue. From the mathematical standpoint of view characteristics of entanglement can be understood within the classical theory of invariants (cf. [3, 4]). The central object in these studies is the ring of G -invariant polynomials, called *local invariants*, in elements of the density matrix with the group G consisting from the so-called *local unitary transformations* acting separately on every part of the multipartite composite system. The program of description of this ring for multipartite mixed states was outlined in [5] and during the last decade has been intensively developed. Over this time many interesting physical and pure mathematical results have been obtained. Particularly, for the simplest bipartite system of two qubits, the structure of the corresponding ring has been clarified (see e.g. [6, 7, 8]). However, comparative less is known for multipartite states, as well as for bipartite mixed states, composed from arbitrary d -level subsystems, the so-called qudits [9, 10]. The reason is first of all in a big computational difficulties we are faced. Indeed, even dealing with 3-level subsystem, qutrit, the large number of independent elements of the density matrix leads to the wide variety of the local polynomial invariants and makes non-effective the direct usage of the modern computer algebra software.

Below, attempting to construct the polynomial ring of local invariants for qubit-qutrit pair, i.e. invariants against the action of $SU(2) \otimes SU(3)$ group, we got added evidence of the complexity of the problem. The known results [12] and our calculation of the Molien function and Poincaré series show that the number of local invariants grows up significantly compared with the two qubits case. Nevertheless the derived information is very useful for the analysis of the polynomial ring of local invariants. As a preliminary result we present here a set of linearly independent local invariants up to the fourth order constructed via trace operation from the non-commutative monomials in three elements of a special decomposition of qubit-qutrit density matrix. Using the subset of the local invariants, consisting from the Casimir invariants

of the enveloping algebra $\mathfrak{U}(\mathfrak{su}(6))$, the positive semi-definiteness of density matrix of qubit-qutrit pair is derived in the form of a system of algebraic inequalities.

2 The $SU(n)$ Casimir invariants

Here the basic statements on the unitary symmetry in quantum mechanics and its role in the description of composite multipartite states is given.

• **Density operator and $SU(n)$ -invariants** • According to the conventional quantum theory, a complete information about a generic n -dimensional system is accumulated in the self-adjoint positive semi-definite density operator ϱ with the unit trace, $\varrho \in \mathfrak{P}_+$. For a closed quantum system, this description is highly redundant, the equivalence relation between elements of \mathfrak{P}_+ , due to the invariance of observables under the adjoint action of $SU(n)$ group

$$(\text{Ad } g)\varrho = g\varrho g^{-1}, \quad g \in SU(n), \quad (2.1)$$

guarantees that the physically relevant knowledge about quantum states can be extracted from the orbit space $\mathfrak{P}_+|SU(n)$ ¹. Relaxing for a moment condition of semi-definiteness, the density operator ϱ can be expressed via the Lie algebra $\mathfrak{su}(n)$ of $SU(n)$ group [11]:

$$\varrho = \frac{1}{n} \mathbb{I}_n + \tilde{\kappa} \imath \mathfrak{g}, \quad \mathfrak{g} \in \mathfrak{su}(n), \quad \imath^2 = -1. \quad (2.2)$$

with some normalization factor $\tilde{\kappa}$. Therefore the density operator can be decomposed over $n^2 - 1$ basis elements, e_i , of the Lie algebra $\mathfrak{su}(n)$

$$\mathfrak{g} = \sum_{i=1}^{n^2-1} \xi_i e_i, \quad (2.3)$$

and any other operator $\mathcal{A}[\varrho]$, constructed from the density operator ρ , admits a representation in the graded power series:

$$\mathcal{A}(\mathbf{e}) = A^{(0)} \mathbb{I} + A_i^{(1)} e_i + \frac{1}{2!} A_{ij}^{(2)} e_i e_j + \frac{1}{3!} A_{ijk}^{(3)} e_i e_j e_k + \dots \quad (2.4)$$

¹The orbit space $\mathfrak{P}_+|SU(n)$ of $SU(n)$ is defined as the set of all $SU(n)$ -orbits, endowed with the quotient topology and differentiable structure, the subset of all the $SU(n)$ -orbits with the same orbit-type forms a stratum of $\mathfrak{P}_+|SU(n)$.

According to the Poincaré-Birkhoff-Witt theorem [13] the ordered monomials

$$e_0 = 1, \quad e_{i_1 i_2 \dots i_k} = e_{i_1} e_{i_2} \dots e_{i_k}, \quad e_{i_1} < e_{i_2} < \dots < e_{i_k}, \quad (2.5)$$

form a linear basis of the universal enveloping algebra $\mathfrak{U}(\mathfrak{su}(n))$ of $\mathfrak{su}(n)$. Direct corollary of this theorem is that the symmetrized monomials of degree d in (2.4) span a linear spaces $\mathfrak{U}^d(\mathfrak{su}(n))$ and the universal enveloping algebra

$$\mathfrak{U}(\mathfrak{su}(n)) = \bigoplus_{d=0}^{\infty} \mathfrak{U}^d(\mathfrak{su}(n)).$$

as a linear space is isomorphic to a polynomial algebra in commutative real variables ξ_i , $i = 1, \dots, n^2 - 1$.

Furthermore, according to the well-known Gelfand's theorem [14], the description of center, $\mathcal{Z}(\mathfrak{su}(n))$, of the enveloping algebra $\mathfrak{U}(\mathfrak{su}(n))$ reduces to the study of invariants in commutative symmetrized algebra $S(\mathfrak{su}(n))$, which is isomorphic to the algebra of invariant polynomials over $\mathfrak{su}(n)$. The elements of center $\mathcal{Z}(\mathfrak{su}(n))$ are in one to one correspondence with the $SU(n)$ -invariant polynomials in $n^2 - 1$ real variables, coordinates in $\mathfrak{su}(n)$. More precisely, the element of $\mathfrak{U}(\mathfrak{su}(n))$

$$\mathfrak{C}_r = \sum_{\sigma \in \mathfrak{S}_r} \frac{1}{r!} c_{i_1 \dots i_r} \sum_{\sigma \in \mathfrak{S}_r} e_{i_{\sigma(1)}} e_{i_{\sigma(2)}} \dots e_{i_{\sigma(r)}},$$

where \mathfrak{S}_r is the group of permutation of $1, 2, \dots, r$, belongs to $\mathcal{Z}(\mathfrak{su}(n))$, if and only if $c_{i_1 \dots i_r}$ are coefficients of the polynomial in $\xi_1, \xi_2, \dots, \xi_r$ variables

$$\phi(\xi_1, \xi_2, \dots, \xi_r) = \sum c_{i_1 \dots i_r} \xi_{i_1} \xi_{i_2} \dots \xi_{i_r},$$

which is invariant under the adjoint action

$$\phi(\xi_1, \xi_2, \dots, \xi_r) = \phi((\text{Ad } g)^T \xi_1, (\text{Ad } g)^T \xi_2, \dots, (\text{Ad } g)^T \xi_r),$$

with $(\text{Ad } g)^T$ - the matrix of adjoint operator, $\text{Ad } g$, calculated in the basis $e_{i_1} e_{i_2} \dots e_{i_r}$.

Therefore, from the algebraic standpoint, the study of the orbit space $\mathfrak{P}_+ | \text{SU}(n)$ as well as any characteristics of quantum-mechanical observables, invariant under the unitary action (2.1), reduces to the computation of the center $\mathcal{Z}(\mathfrak{su}(n))$ of $\mathfrak{U}(\mathfrak{su}(n))$.

If the elements \mathfrak{C}_r belong to \mathcal{Z} they are termed as Casimir operators. The number of independent homogeneous Casimir generators for $SU(n)$ group is equal to rank $\mathfrak{su}(n) = n - 1$.

It is well known, that the quadratic Casimir operator is unique up to the constant factor and is expressible with the aid of the Cartan tensor:

$$C_{ij} = \text{tr}((\text{Ad } e_i)(\text{Ad } e_j)),$$

Therefore for algebra $\mathfrak{su}(n)$ the quadratic Casimir operator reads

$$\mathfrak{C}_2 = \sum e_i e_i,$$

The higher dimensional Casimirs are expressed via the symmetric structure constants d_{ijk} of $\mathfrak{su}(n)$ algebra [15]. Because further, dealing with the qubit-qutrit system the Casimirs of $SU(6)$ will be used ², the expressions for \mathfrak{C}_i are given below:

$$\begin{aligned} \mathfrak{C}_3 &= \sum d_{i_1 i_2 i_3} e_{i_1} e_{i_2} e_{i_3}, \\ \mathfrak{C}_4 &= \sum d_{j i_1 i_2} d_{j i_3 i_4} e_{i_1} e_{i_2} e_{i_3} e_{i_4}, \\ \mathfrak{C}_5 &= \sum d_{i_1 i_2} d_{i_3 i_4} d_{j i_4 i_5} e_{i_1} e_{i_2} e_{i_3} e_{i_4} e_{i_5} e_{i_6}, \\ \mathfrak{C}_6 &= \sum d_{i_1 i_2} d_{i_3 i_4} d_{j k i_4} d_{k i_5 i_6} e_{i_1} e_{i_2} e_{i_3} e_{i_4} e_{i_5} e_{i_6}. \end{aligned}$$

Now using these operators and decomposition (2.3) based on the isomorphism between center $\mathcal{Z}(\mathfrak{su}(n))$ and $SU(n)$ -invariant polynomials, the following scalars, referred hereafter as Casimir invariants, can be written:

$$\mathfrak{C}_2 = (n - 1) \boldsymbol{\xi} \cdot \boldsymbol{\xi} \quad (2.6)$$

$$\mathfrak{C}_3 = (n - 1) (\boldsymbol{\xi} \vee \boldsymbol{\xi}) \cdot \boldsymbol{\xi} \quad (2.7)$$

$$\mathfrak{C}_4 = (n - 1) (\boldsymbol{\xi} \vee \boldsymbol{\xi}) \cdot (\boldsymbol{\xi} \vee \boldsymbol{\xi}) \quad (2.8)$$

$$\mathfrak{C}_5 = (n - 1) \left((\boldsymbol{\xi} \vee \boldsymbol{\xi}) \vee (\boldsymbol{\xi} \vee \boldsymbol{\xi}) \right) \cdot \boldsymbol{\xi} \quad (2.9)$$

$$\mathfrak{C}_6 = (n - 1) (\boldsymbol{\xi} \vee \boldsymbol{\xi} \vee \boldsymbol{\xi})^2 \quad (2.10)$$

where

$$(\mathbf{U} \vee \mathbf{V})_a := \kappa d_{abc} U_b V_c,$$

²The tensorial $\mathfrak{su}(2) \otimes \mathfrak{su}(3)$ product type basis for $\mathfrak{su}(6)$ is given in Appendix A. The formulas for the symmetric structure constants d_{ijk} and the antisymmetric structure constants f_{ijk} for $\mathfrak{su}(n)$ are presented there as well.

with normalization constant $\kappa := \sqrt{n(n-1)/2}$.

Now, using these scalars, the positive semi-definiteness of density matrices for an arbitrary n -level quantum system will be formulated.

• **Positivity of density operators** • To the best of our knowledge the first analysis of consequences of the constraints on the density operator due to its semi-positive definiteness has been done in the sixtieth of the last century studying the production and decay of resonant states in strong interaction processes [16, 17, 18]. Nowadays, the quantum computing and theory of quantum information reveals the new role of these constraints and recently they have been once more derived [19, 20]³.

To formulate the semi-definiteness let us choose the Bloch representation for a density operator (2.2) [11]:

$$\varrho = \frac{1}{n} (\mathbb{I}_n + \omega), \quad \omega = \kappa \boldsymbol{\xi} \cdot \boldsymbol{\lambda}, \quad (2.11)$$

where $(n^2 - 1)$ -dimensional Bloch vector $\boldsymbol{\xi} \in \mathbb{R}^{n^2-1}$ is contracted with elements λ_i , $i = 1, \dots, n^2 - 1$ of the Hermitian basis of $\mathfrak{su}(n)$ Lie algebra. According to [17]⁴ a necessary and sufficient condition for the Hermitian matrix to be positive is that the coefficients S_k of its characteristic equation

$$|\mathbb{I}x - \varrho| = x^n - S_1x^{n-1} + S_2x^{n-2} - \dots + (-1)^n S_n = 0 \quad (2.12)$$

should be non-negative

$$\varrho \geq 0 \Leftrightarrow S_k \geq 0 \quad k = 1, \dots, n. \quad (2.13)$$

It is convenient to rewrite these inequalities in terms of normalized coefficients $\bar{S}_k := S_k / \max\{S_k\}$. Since the maximal values of S_k correspond to a maximally degenerate roots; $x_1 = x_2 = \dots = x_n = 1/n$ of the characteristic equation (2.12) one can express them via the binomial coefficients

$$\max\{S_k\} = \frac{1}{n^k} \binom{n}{n-k}$$

and thus

$$0 \leq \bar{S}_k \leq 1 \quad k = 2, \dots, n. \quad (2.14)$$

³In our recent publication [8] the positivity conditions for density operators has been analyzed in context of the consequences for integrity basis of $SU(2) \otimes SU(2)$ polynomial invariants ring as well as for entanglement characteristics of mixed qubit states [21].

⁴Note that P.Minnaert attributed the same result to D.N.Williams.

Now we are ready to rewrite the constraints (2.14) in terms of the Casimir invariants (2.6)-(2.10). This is possible since, each of three sets, \mathfrak{C}_k , or S_k , or $t_k = \text{tr}(\varrho^k)$, $k = 2, \dots, n$ forms the basis of algebraically independent invariants of $\text{SU}(n)$ group (see e.g. [15]). The expressions for the coefficients S_k in terms of t_m are well-known, they are given by determinants:

$$S_k = \frac{1}{k!} \begin{vmatrix} t_1 & 1 & 0 & 0 & \cdots & 0 \\ t_2 & t_1 & 2 & 0 & \cdots & 0 \\ t_3 & t_2 & t_1 & 3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ t_{k-1} & t_{k-2} & t_{k-3} & t_{k-4} & \cdots & k-1 \\ t_k & t_{k-1} & t_{k-2} & t_{k-3} & \cdots & t_1 \end{vmatrix}.$$

Further, t_m can be represented as polynomials in Casimir invariants. Based on the expressions for traces of symmetrized products of Lie algebra basis elements (see Appendix A, cf. also [20]) we have:

$$\begin{aligned} \text{tr}(\omega^2) &= n\mathfrak{C}_2, \\ \text{tr}(\omega^3) &= n\mathfrak{C}_3, \\ \text{tr}(\omega^4) &= n(\mathfrak{C}_2^2 + \mathfrak{C}_4), \\ \text{tr}(\omega^5) &= n(2\mathfrak{C}_2\mathfrak{C}_3 + \mathfrak{C}_5), \\ \text{tr}(\omega^6) &= n(\mathfrak{C}_2^3 + 2\mathfrak{C}_2\mathfrak{C}_4 + \mathfrak{C}_3^2 + \mathfrak{C}_6). \end{aligned}$$

Finally, imposing the following normalization for the Casimir invariants,

$$C_k = \frac{(k-1)!}{(n-1)(n-2)\dots(n-k+1)} \mathfrak{C}_k,$$

we arrive at a system of inequalities in $\text{su}(6)$ Casimir invariants, that defines the positive semi-definiteness of the density matrix of qubit-qutrit pair:

$$0 \leq C_2 \leq 1, \quad (2.15)$$

$$0 \leq 3C_2 - C_3 \leq 1, \quad (2.16)$$

$$0 \leq 6C_2 - 5C_2^2 - 4C_3 + C_4 \leq 1, \quad (2.17)$$

$$0 \leq (1 - 5C_2)^2 - 30C_2C_3 + 10C_3 - 5C_4 + C_5 \leq 1 \quad (2.18)$$

$$\begin{aligned} 0 \leq & (1 - 5C_2)^3 - 180C_2C_3 + 125C_2C_4 + \\ & + 20C_3(1 + 5C_3) - 15C_4 + 6C_5 - C_6 \leq 1. \end{aligned} \quad (2.19)$$

Since the positive semi-definiteness of density matrices plays an exceptional role in the entanglement quantification problem it is reasonable to rewrite the system of inequalities (2.15)-(2.19) in terms of the local $SU(2) \otimes SU(3)$ invariants.

3 The local unitary invariants

• **The local invariance of composite states** • When a quantum system is obtained by combining of r -subsystems with n_1, n_2, \dots, n_r levels each, the non-local properties of the composite system are in correspondence with a certain decomposition of the unitary operations (2.1).

In order to discuss this decomposition consider the subgroup of unitary group formed by the *local unitary transformations*

$$SU(n_1) \otimes SU(n_2) \otimes \cdots \otimes SU(n_r), \quad (3.1)$$

acting independently on the density matrix of each subsystem

$$\varrho^{(n_i)} \rightarrow \varrho^{(n_i)'} = g \varrho^{(n_i)} g^{-1} \quad g \in SU(n_i), \quad i = 1, 2, \dots, r.$$

Two states of composite system connected by the local unitary transformations (3.1) have the same non-local properties. The latter can be changed only by the rest of the unitary actions,

$$\frac{SU(n)}{SU(n_1) \otimes SU(n_2) \otimes \cdots \otimes SU(n_r)}, \quad n = n_1 n_2 \cdots n_r,$$

generating the class of non-local transformations.

Having this notions, we are in position to discuss the structure of the corresponding ring of polynomial local invariants, i.e. polynomials in elements of the density matrices, which are scalars under the adjoint local unitary transformations. It is well known that for any reductive linear algebraic group G and for any finite dimensional G -module V , the ring \mathcal{R}^G has the Cohen-Macaulay property [22] and possesses the Hironaka decomposition

$$\mathcal{R}^G = \bigoplus_{a=0}^r J_a \mathbb{C}[K_1, K_2, \dots, K_s],$$

where $K_b, b = 1, 2, \dots, s$ are primary, algebraically independent polynomials and $J_a, a = 0, 1, 2, \dots, r, J_0 = 1$, are secondary, linearly independent invariants respectively. According to that the corresponding Molien function $M_G(q)$ for \mathcal{R}^G [7] can be expressed as follows

$$M_G(q) = \frac{\sum_{a=0}^r q^{\deg J_a}}{\prod_{b=1}^s (1 - q^{\deg K_b})}.$$

In this form it provides us with a certain knowledge on the numbers of algebraically independent polynomials as well as linearly independent invariants.

• **Molien functions for $\mathbb{C}[\mathfrak{P}_+^{(2\otimes 2)}]$ and $\mathbb{C}[\mathfrak{P}_+^{(2\otimes 3)}]$** • Let us start with a remark concerning the adjoint action (2.1). Consider a non-degenerate density matrices. In this case using the natural identification of the elements of a linear space spanned by the Hermitian $n \times n$ matrices with the space \mathbb{R}^{n^2-1}

$$\varrho \rightarrow \rho_{ij}$$

one can instead of the adjoint action (2.1) consider the linear representation on \mathbb{R}^{n^2-1}

$$V'_A = L_{AB} V_B, \quad L_{AB} \in \mathrm{SU}(n) \otimes \overline{\mathrm{SU}(n)},$$

where the line over expression means the complex conjugation.

After this identification in order to get some insight on the structure of the ring of polynomial invariants of linear action of Lie group G on the linear V space we can compute the Molien function

$$M(\mathbb{C}[V]^G, q) = \int_G \frac{d\mu(g)}{\det(\mathbb{I} - q\pi(g))}, \quad |q| < 1, \quad (3.2)$$

where $d\mu(g)$ is the Haar measure for Lie group G and $\pi(g)$ is the corresponding representation on V . We start with the system of two qubits.

Two qubits. In this case the local unitary group is

$$G = \mathrm{SU}(2) \otimes \mathrm{SU}(2).$$

As it is well known for any reductive linear group the integration in (3.2) reduces to the integration over the maximal compact subgroup K of G [4]. In the present case this results in integration over the maximal torus

$$\pi(g) = \mathrm{diag}(1, 1, z, z^{-1}) \otimes \mathrm{diag}(1, 1, w, w^{-1}),$$

where z, w - coordinates on one-dimensional tori. Therefore computations reduce to the following two-dimensional integral

$$M_{\text{SU}(2) \otimes \text{SU}(2)}(q) = \frac{1}{(2\pi i)^2} \int_{|z|=1} \int_{|w|=1} \frac{d\mu}{\Psi(z, w, q)},$$

where

$$\begin{aligned} d\mu &= (1-z)^2(1-w)^2 \frac{dz}{z^2} \frac{dw}{w^2}, \\ \det(\mathbb{I} - q\pi(g)) &= (1-q)\Psi(z, w, q) \\ \Psi(z, w, q) &= (1-q)^3(1-qz)^2(1-qw)^2(1-qz^{-1})^2(1-qw^{-1})^2 \\ &\quad (1-qzw)(1-qz^{-1}w)(1-qzw^{-1})(1-qz^{-1}w^{-1}). \end{aligned}$$

After integration we get the Molien function [7]

$$M_{\text{SU}(2) \otimes \text{SU}(2)}(q) = \frac{1 + q^4 + q^5 + 3q^6 + 2q^7 + 2q^8 + 3q^9 + q^{10} + q^{11} + q^{15}}{(1-q^2)^3(1-q^3)^2(1-q^4)^3(1-q^6)},$$

which is the palindromic one,

$$M_{\text{SU}(2) \otimes \text{SU}(2)}(1/q) = -q^{15}M_{\text{SU}(2) \otimes \text{SU}(2)}(q),$$

with the degree consistent with

$$\dim \text{SU}(4) = 15.$$

Qubit-Qutrit. Now the local unitary group is $G = \text{SU}(2) \otimes \text{SU}(3)$ and owing to the symmetries of the integrand (3.2) the non-trivial part of the integration is entirely accumulated in the diagonal components of the $\pi(g)$ -representation of the form:

$$\pi(g)_{\text{diag}} = \text{diag}(1, 1, x, x^{-1}) \otimes \text{diag}(1, 1, 1, y, z, yz, y^{-1}, z^{-1}, (yz)^{-1}),$$

where x, y and z are coordinates on the maximal torus. Therefore, the computation of the Molien function (3.2) reduces to the evaluation of the multiple contour integral in complex planes over unit circles ⁵:

$$M_{\text{SU}(2) \otimes \text{SU}(3)}(q) = \frac{1}{(2\pi i)^3} \int_{|x|=1} \int_{|y|=1} \int_{|z|=1} f(x, y, z, q) dx dy dz, \quad (3.3)$$

⁵The multiple integral (3.3) has been calculated using the consecutive application of Cauchy's residue theorem. Since the integrand f has poles of rather high orders, computer computations of the residues has been performed using the command `Residue` built-in Mathematica that implements the standard limit formula for high order poles (see <http://mathworld.wolfram.com/ComplexResidue.html>).

where

$$f(x, y, z, q) = \frac{1}{xyz} \frac{(1 - x^{-1})(1 - y^{-1})(1 - z^{-1})(1 - (yz)^{-1})}{\Psi(x, y, z, q)},$$

$$\det(\mathbb{I} - q\pi(g)) = (1 - q)\Psi(x, y, z, q),$$

and $\Psi(x, y, z, q) =$

$$\begin{aligned} & (1 - q)^5(1 - qy)^2(1 - qz)^2(1 - qyz)^2(1 - \frac{q}{y})^2(1 - \frac{q}{z})^2(1 - \frac{q}{yz})^2 \\ & (1 - qx)^3(1 - qxy)(1 - qxz)(1 - qxyz)(1 - \frac{qx}{y})(1 - \frac{qx}{z})(1 - \frac{qx}{yz}) \\ & (1 - \frac{q}{x})^3(1 - \frac{qy}{x})(1 - \frac{qz}{x})(1 - \frac{qyz}{x})(1 - \frac{q}{xy})(1 - \frac{q}{xz})(1 - \frac{q}{xyz}). \end{aligned}$$

As a result, the Molien function can be represented in the rational form (cf. [12]):

$$M_{\text{SU}(2) \otimes \text{SU}(3)}(q) = \frac{N}{D}, \quad (3.4)$$

where

$$\begin{aligned} N = & 1 + 4q^4 + 9q^5 + 38q^6 + 69q^7 + 173q^8 + 347q^9 + 733q^{10} + 1403q^{11} \\ & + 2796q^{12} + 5091q^{13} + 9286q^{14} + 16058q^{15} + 27208q^{16} + 44250q^{17} \\ & + 70537q^{18} + 108430q^{19} + 163158q^{20} + 238264q^{21} + 339974q^{22} \\ & + 472130q^{23} + 641187q^{24} + 848615q^{25} + 1098643q^{26} + 1388741q^{27} \\ & + 1717327q^{28} + 2075836q^{29} + 2456389q^{30} + 2843020q^{31} + 3222408q^{32} \\ & + 3575226q^{33} + 3884797q^{34} + 4133599q^{35} + 4308636q^{36} + 4398377q^{37} \\ & + 4398377q^{38} + \dots + 38q^{69} + 9q^{70} + 4q^{71} + q^{75} \\ D = & (1 - q^2)^3(1 - q^3)^4(1 - q^4)^5(1 - q^5)^4(1 - q^6)^5(1 - q^7)^2(1 - q^8). \end{aligned}$$

This Molien function is the palindromic one

$$M_{\text{SU}(2) \otimes \text{SU}(3)}(1/q) = q^{35}M_{\text{SU}(2) \otimes \text{SU}(3)}(q),$$

as provided by

$$\dim \text{SU}(6) = 35.$$

This form of the Molien function serves as source of information on the polynomial ring of $\text{SU}(2) \otimes \text{SU}(3)$ invariants. Particularly, one can endeavour

to identify the structure of algebraically independent local unitary scalars. According to (3.4) there are 24 independent scalars in agreement with simple count of $\dim [\mathrm{SU}(6)/\mathrm{SU}(2) \otimes \mathrm{SU}(3)] = 35 - 11 = 24$. The set of these 24 polynomial invariants may be composed from three invariants of degree 2, four of degree 3, five of degree 4, four of degree 5, five of degree 6, two of degree 7 and one of the degree 8.

Note that the Poincaré series of $M_{\mathrm{SU}(2) \otimes \mathrm{SU}(3)}(q)$

$$M_{\mathrm{SU}(2) \otimes \mathrm{SU}(3)}(q) = \sum_{d=0}^{\infty} \dim \left(\mathcal{P}_d^{\mathrm{SU}(2) \otimes \mathrm{SU}(3)} \right) q^d,$$

determines the number of homogeneous polynomial invariants of degree d . According to the calculations of (3.3) the few terms of the Taylor expansion over q are

$$\begin{aligned} M_{\mathrm{SU}(2) \otimes \mathrm{SU}(3)}(q) = & 1 + 3q^2 + 4q^3 + 15q^4 + 25q^5 + 90q^6 + 170q^7 + 489q^8 \\ & + 1059q^9 + 2600q^{10} + 5641q^{11} + 12872q^{12} + 27099q^{13} \\ & + 57990q^{14} + 118254q^{15} + 240187q^{16} + O(q^{17}). \end{aligned} \quad (3.5)$$

Now, having in mind the input from the structure of the Molien function (3.4), we attempt to construct the local $\mathrm{SU}(2) \otimes \mathrm{SU}(3)$ unitary invariants.

• **Constructing $\mathrm{SU}(2) \otimes \mathrm{SU}(3)$ invariants** • Let us introduce the decomposition for density matrices well adapted to the case of composite qubit-qutrit system. The space $\mathfrak{su}(6)$ in (2.2) for $n=6$ admits decomposition in the direct sum of three real spaces

$$\mathfrak{su}(6) = \bigoplus_{a=1}^3 V_a = \mathfrak{su}(2) \otimes \mathbb{I}_3 + \mathbb{I}_2 \otimes \mathfrak{su}(2) + \mathfrak{su}(2) \otimes \mathfrak{su}(3).$$

Using Pauli matrices σ_i as the basis for $\mathfrak{su}(2)$ and Gell-Mann matrices λ_a as the basis for $\mathfrak{su}(3)$ (see Appendix A) the density matrix (2.11) for qubit-qutrit system can be written as [9, 10]:

$$\varrho = \frac{1}{6} [\mathbb{I}_6 + \omega], \quad \omega = \alpha + \beta + \gamma,$$

where

$$\alpha := \sum_{i=1}^3 a_i \sigma_i \otimes \mathbb{I}_3, \quad \beta := \sum_{a=1}^8 b_a \mathbb{I}_2 \otimes \lambda_a, \quad \gamma := \sum_{i=1}^3 \sum_{a=1}^8 c_{ia} \sigma_i \otimes \lambda_a.$$

Among the $35=3+8+24$ real parameters (a_i, b_a, c_{ia}) the first two sets, a_i and b_a , correspond to the Bloch vectors of an individual qubit and qutrit respectively; the evaluation of partial trace yields the reduced matrices for subsystems:

$$\varrho^{(A)} := \text{tr}_B(\varrho) = \frac{1}{2}(\mathbb{I}_2 + \vec{a} \cdot \vec{\sigma}), \quad \varrho^{(B)} := \text{tr}_A(\varrho) = \frac{1}{3}(\mathbb{I}_3 + \vec{b} \cdot \vec{\lambda}),$$

while the variables c_{ia} are entries of the so-called correlation matrix $C = (c_{ia})$.

Now using a trace operation described below we can construct a set of local $\text{SU}(2) \otimes \text{SU}(3)$ scalars, candidates for the elements of the integrity basis.

In analogy with the generators (2.5) of the universal enveloping algebra we consider a set \mathcal{M} of non-commutative monomials

$$\mathcal{M}_{i_1 \dots i_d} := X_{i_1} \cdot X_{i_2} \cdot \dots \cdot X_{i_d} \in \mathcal{M},$$

where each of X_{i_k} , $k = 1, \dots, d$, is one of α, β , or γ . To each $\mathcal{M}_{i_1 \dots i_d}$ we assign a multidegree (s, t, q) , $s + t + q = d$, where s, t and q are degrees of α, β , and γ respectively. The trace operation on monomials $\mathcal{M}_{i_1 \dots i_d}$

$$\text{tr} : \mathcal{M}_{i_1 \dots i_d} \rightarrow \mathcal{P}_{stq}(a_i, b_a, c_{ia}) := \text{tr}(\mathcal{M}_{i_1 \dots i_d}) \in \mathcal{P}.$$

defines the map $\text{tr} : \mathcal{M} \rightarrow \mathcal{P}$ of \mathcal{M} into the algebra \mathcal{P} of homogeneous polynomials in variables (a_i, b_a, c_{ia}) . A generic term of the polynomial $\mathcal{P}_{stq}(a_i, b_a, c_{ia})$ is a convolution of vectors a_i, b_a and matrix c_{ia} with traces

$$\text{tr}(\sigma_1 \sigma_2 \cdots \sigma_p \otimes \lambda_1 \lambda_2 \cdots \lambda_r) = \text{tr}(\sigma_1 \sigma_2 \cdots \sigma_p) \text{tr}(\lambda_1 \lambda_2 \cdots \lambda_r),$$

where $p = s + q$ and $r = t + q$.

Now it is easy to verify that the images of the trace map are local unitary invariants. Indeed, since under the transformation of the form $k_1 \otimes k_2$, where $k_1 \in \text{SU}(2)$, and $k_2 \in \text{SU}(3)$, the matrices σ 's and λ 's in the basis elements of $\mathfrak{su}(6)$ (see Appendix A) are transformed independently, in adjoint manner

$$\sigma \rightarrow k_1 \sigma k_1^{-1}, \quad \lambda \rightarrow k_2 \lambda k_2^{-1},$$

the polynomials $\text{tr}(\mathcal{M})$ are invariant against $\text{SU}(2) \otimes \text{SU}(3)$ action.

Therefore the polynomials $\mathcal{P}_{stq}(a_i, b_a, c_{ia})$ are the reserve for the integrity basis of the ring $\mathbb{C}[\mathfrak{P}]^{\text{SU}(2) \otimes \text{SU}(3)}$. Now, in contrast to the case of $\text{SU}(n)$ Casimir invariants built up with the help of symmetric structure constants

only, dealing with the scalars against the tensor product of groups, the invariants are constructed in terms of the antisymmetric structure constants as well. For example,

$$\text{tr}(\gamma^3) = c_{ia}c_{jb}c_{kc}\text{tr}(\sigma_i\sigma_j\sigma_k \otimes \lambda_a\lambda_b\lambda_c) = c_{ia}c_{jb}c_{kc}\text{tr}(\sigma_i\sigma_j\sigma_k) \text{tr}(\lambda_a\lambda_b\lambda_c) .$$

This quantity being invariant under the $SU(2) \otimes SU(3)$ action is expressible via totally antisymmetric tensor ϵ_{ijk} - structure constants of $\mathfrak{su}(2)$ algebra and f_{abc} - structure constants of $\mathfrak{su}(3)$:

$$\text{tr}(\gamma^3) = -4\epsilon_{ijk}f_{abc}c_{ia}c_{jb}c_{kc} .$$

Choosing a basis for local invariants, several types of algebraic dependence between the polynomials in \mathcal{P} have to be taken into account. It is worth to consider two illustrative examples. Applying the Hamilton-Cayley theorem for elements α, β and γ , considered as Hermitian 6×6 matrices, one can determine the algebraic identities for the polynomials of the degree $d > 7$. Less obvious example of relations between polynomials is due to the identities between the structure constants of the algebra.⁶ Let us consider two invariants, both 4-th order in variables c_{ia} of the correlation matrix C , but one constructed using the invariant symmetric structure constants d while the second one with the anti-symmetric structure constants f :

$$\begin{aligned} \mathfrak{I}^{004}(dd) &= d_{abc}d_{cpq}(C^T C)_{ab}(C^T C)_{pq} , \\ \mathfrak{I}^{004}(ff) &= f_{apc}f_{cbq}(C^T C)_{ab}(C^T C)_{pq} . \end{aligned}$$

With the aid of identities (A.1) and (A.2) (Appendix A) for the structure constants of $\mathfrak{su}(3)$ algebra, one can convinced that

$$\mathfrak{I}^{004}(dd) = \frac{2}{3}\mathfrak{I}^{004}(ff) - \frac{1}{3}\left[\left(\text{tr}(C^T C)\right)^2 - 2\text{tr}(C^T C C^T C)\right] .$$

According to the Poincaré series (3.5) there are 15 homogeneous scalars of order 4, while there are $81 = 3^4$ monomials in three noncommutative variables. But since the elements α and β commute this number reduces. Taking into account this commutativity as well as the invariance of trace operation under the cyclic permutations of products, one can find 18 valuable

⁶For the detailed analysis of the relations of that type we refer to [23].

monomials:

$$\begin{aligned} & \alpha^4, \beta^4, \gamma^4, \alpha^3\beta, \alpha\beta^3, \alpha^3\gamma, \alpha\gamma^3, \beta^3\gamma, \beta\gamma^3, \\ & \alpha^2\beta^2, \alpha^2\gamma^2, \alpha\gamma\alpha\gamma, \beta^2\gamma^2, \beta\gamma\beta\gamma, \\ & \alpha^2\beta\gamma, \alpha\beta^2\gamma, \alpha\beta\gamma^2, \alpha\gamma\beta\gamma. \end{aligned}$$

Taking traces of these monomials one can convince that five of them form the kernel of trace map:

$$\text{tr}(\alpha^3\beta) = \text{tr}(\alpha\beta^3) = \text{tr}(\alpha^3\gamma) = \text{tr}(\beta^3\gamma) = \text{tr}(\alpha^2\beta\gamma) = 0,$$

and images of last two monomials coincide up to sign

$$\text{tr}(\alpha\beta\gamma^2) = -\text{tr}(\alpha\gamma\beta\gamma).$$

Therefore the following set of twelve traces

$$\begin{aligned} & \text{tr}(\alpha^4), \text{tr}(\beta^4), \text{tr}(\alpha^2\beta^2), \text{tr}(\alpha^2\gamma^2), \\ & \text{tr}(\gamma^4), \text{tr}(\alpha\gamma^3), \text{tr}(\beta\gamma^3), \text{tr}(\alpha\gamma\alpha\gamma), \\ & \text{tr}(\beta^2\gamma^2), \text{tr}(\beta\gamma\beta\gamma), \text{tr}(\alpha\beta^2\gamma), \text{tr}(\alpha\beta\gamma^2), \end{aligned}$$

plus three 4-th order polynomials constructed as products of second degrees polynomials $\text{tr}(\alpha^2)\text{tr}(\beta^2)$, $\text{tr}(\alpha^2)\text{tr}(\gamma^2)$, $\text{tr}(\beta^2)\text{tr}(\gamma^2)$, are 15 homogeneous invariant polynomials in accordance with the Poincaré series (3.5).

How difficult is it to extract the independent scalars from this list? It is easy to verify that some traces are expressed in terms polynomials of second order; e.g., $\text{tr}(\alpha^2\beta^2) = \frac{1}{6}\text{tr}(\alpha^2)\text{tr}(\beta^2)$. Concerning the remaining monomials one can see that several of them have the same multidegree. Namely, the following “trace” polynomials

1. $\text{tr}(\alpha^2\gamma^2) = \frac{1}{6}\text{tr}(\alpha^2)\text{tr}(\gamma^2)$ and $\text{tr}(\alpha\gamma\alpha\gamma)$,
2. $\text{tr}(\beta^2)\text{tr}(\gamma^2)$, $\text{tr}(\beta^2\gamma^2)$ and $\text{tr}(\beta\gamma\beta\gamma)$,

belong to the same space \mathcal{P}_{202} and \mathcal{P}_{022} respectively. Being linearly independent monomials, they obey the following relations

$$\begin{aligned} & \text{tr}(\alpha^2\gamma^2) + \text{tr}(\alpha\gamma\alpha\gamma) = 8a_{i_1}a_{i_2}c_{i_1j_1}c_{i_2j_1}, \\ & \text{tr}(\beta^2\gamma^2) - \frac{1}{6}\text{tr}(\beta^2)\text{tr}(\gamma^2) = 4d_{j_1j_2k}d_{k j_3 j_4}b_{j_1}b_{j_2}c_{i_1j_3}c_{i_1j_4}, \\ & \text{tr}(\beta^2\gamma^2) + \text{tr}(\beta\gamma\beta\gamma) = 8(\frac{2}{3}b_{j_1}b_{j_2}c_{i_1j_1}c_{i_1j_2} + d_{j_1j_2k}d_{k j_3 j_4}b_{j_1}b_{j_3}c_{i_1j_2}c_{i_1j_4}), \end{aligned}$$

where summation over all indices is assumed. This circumstance leaves an open question how to build the elements of integrity basis with a certain multidegree using the “trace” polynomials.

We resume our analysis by the following list of linearly independent $SU(2) \otimes SU(3)$ scalars which are not products of low orders ones ⁷:

- degree 2, three invariants

$$\text{tr}(\alpha^2), \text{tr}(\beta^2), \text{tr}(\gamma^2),$$

- degree 3, four invariants

$$\text{tr}(\beta^3), \text{tr}(\gamma^3), \text{tr}(\alpha\beta\gamma), \text{tr}(\beta\gamma^2),$$

- degree 4, eight invariants

$$\begin{aligned} \text{tr}(\gamma^4), \text{tr}(\alpha\gamma^3), \text{tr}(\beta\gamma^3), \text{tr}(\alpha\gamma\alpha\gamma), \\ \text{tr}(\beta^2\gamma^2), \text{tr}(\beta\gamma\beta\gamma), \text{tr}(\alpha\beta^2\gamma), \text{tr}(\alpha\beta\gamma^2). \end{aligned}$$

• **Casimir invariants decomposition** • The expansion of the $SU(6)$ Casimir invariants up to the 4-th order (2.6)-(2.8) over the above suggested $SU(2) \otimes SU(3)$ “trace” scalars reads:

$$\begin{aligned} 6\mathfrak{C}_2 &= \text{tr}(\alpha^2) + \text{tr}(\beta^2) + \text{tr}(\gamma^2), \\ 6\mathfrak{C}_3 &= \text{tr}(\beta^3) + \text{tr}(\gamma^3) + 3\text{tr}(\beta\gamma^2) + 6\text{tr}(\alpha\beta\gamma), \\ 6\mathfrak{C}_4 &= \frac{1}{3} \left[\text{tr}(\alpha^2) \left(2\text{tr}(\beta^2) + \text{tr}(\gamma^2) \right) + \frac{1}{4} \text{tr}(\beta^2)^2 - \frac{1}{2} \text{tr}(\gamma^2)^2 - \text{tr}(\beta^2)\text{tr}(\gamma^2) \right] \\ &\quad + 4 \left[\text{tr}(\alpha\gamma^3) + \text{tr}(\beta\gamma^3) + \text{tr}(\beta^2\gamma^2) + \text{tr}(\alpha\beta\gamma^2) + 3\text{tr}(\alpha\beta^2\gamma) \right] \\ &\quad + 2 \left[\text{tr}(\alpha\gamma\alpha\gamma) + \text{tr}(\beta\gamma\beta\gamma) \right] + \text{tr}(\gamma^4). \end{aligned}$$

We conclude with the final remark on the applicability of the derived results to the problem of classification of mixed quantum states. Using inequalities (2.15)-(2.19) and results from [21] the well-known Peres—Horodecki criterion for the separability of qubit-qutrit mixed states can be reformulated as a set of inequalities in $SU(2) \otimes SU(3)$ scalars.

⁷Note that 2-nd and 3-d order invariants were proposed in [12].

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A Appendix: Formulas for the $\mathfrak{su}(6)$ algebra

• **The tensorial basis** • For the $\mathfrak{su}(6)$ algebra we use the basis $\{\tau_A\}_{A=1,\dots,35}$ constructed from the tensor products of the Pauli matrices $\sigma_i \in \mathfrak{su}(2)$:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and eight $\{\lambda_a\}_{a=1,\dots,8}$ Gell-Mann matrices, forming the $\mathfrak{su}(3)$ basis:

$$\begin{aligned} \lambda_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} & \lambda_2 &= \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} & \lambda_3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ \lambda_4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} & \lambda_5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} & \lambda_6 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \\ \lambda_7 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} & \lambda_8 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \end{aligned}$$

The elements τ_A are enumerated as

$$\begin{aligned} \tau_i &= \frac{1}{\sqrt{3}} \sigma_i \otimes \mathbb{I}_3, & \tau_{3+a} &= \frac{1}{\sqrt{2}} \mathbb{I}_2 \otimes \lambda_a, \\ \tau_{11+a} &= \frac{1}{\sqrt{2}} \sigma_1 \otimes \lambda_a, & \tau_{19+a} &= \frac{1}{\sqrt{2}} \sigma_2 \otimes \lambda_a, & \tau_{27+a} &= \frac{1}{\sqrt{2}} \sigma_3 \otimes \lambda_a. \end{aligned}$$

• **The algebraic structures** • The product of basis elements reads

$$\tau_A \tau_B = \frac{2}{n} \delta_{AB} \mathbb{I} + (d_{ABC} + i f_{ABC}) \tau_C,$$

The structure constants d_{ABC} and f_{ABC} can be determined via equations

$$d_{ABC} = \frac{1}{4} \text{Tr}(\{\tau_A, \tau_B\} \tau_C), \quad f_{ABC} = -\frac{i}{4} \text{Tr}([\tau_A, \tau_B] \tau_C),$$

where apart from the Lie algebra product, $[,]$, the “anti-commutator” of elements, i.e., $\{\tau_A, \tau_B\} = \tau_A \tau_B + \tau_B \tau_A$ has been used.

• **Identities for structure constants** • For the $SU(n)$ group the the structure constants obey the following identities:

$$\begin{aligned} f_{abc} f_{cpq} + f_{bpc} f_{caq} + f_{pac} f_{cbq} &= 0, \\ d_{abc} f_{cpq} + d_{bpc} f_{caq} + d_{pac} f_{cbq} &= 0, \\ f_{abc} f_{cpq} = d_{apc} d_{cbq} - d_{aqc} d_{cbp} + \frac{2}{n} (\delta_{ap} \delta_{bq} - \delta_{aq} \delta_{bp}), \\ f_{abc} f_{cpq} + f_{aqc} f_{cpb} &= 2d_{apc} d_{cbq} - d_{abc} d_{cpq} - d_{aqc} d_{cbp} \\ &+ \frac{2}{n} (2\delta_{ap} \delta_{bq} - \delta_{ab} \delta_{pq} - \delta_{aq} \delta_{bp}). \end{aligned} \quad (A.1)$$

The $SU(3)$ symmetric constants satisfy [24, 25] an important identities

$$d_{abc} d_{cpq} + d_{bpc} d_{caq} + d_{pac} d_{cbq} = \frac{1}{3} (\delta_{ab} \delta_{pq} + \delta_{ap} \delta_{bq} + \delta_{aq} \delta_{bp}). \quad (A.2)$$

• **The traces** • The traces of symmetrized products of $\mathfrak{su}(n)$ basis elements are

$$\begin{aligned} \text{tr}(\tau_{\{a} \tau_{b\}}) &= 2\delta_{ab}, \\ \text{tr}(\tau_{\{a} \tau_b \tau_{c\}}) &= 2d_{abc}, \\ \text{tr}(\tau_{\{a} \tau_b \tau_c \tau_{d\}}) &= \frac{2^2}{n} \delta_{ab} \delta_{cd} + 2d_{abe} d_{ecd}, \\ \text{tr}(\tau_{\{a} \tau_b \tau_c \tau_d \tau_{e\}}) &= \frac{2^2}{n} (d_{abc} \delta_{de} + \delta_{ab} d_{cde}) + 2d_{abf} d_{fcg} d_{gde}, \\ \text{tr}(\tau_{\{a} \tau_b \tau_c \tau_d \tau_e \tau_{f\}}) &= \frac{2^3}{n^2} \delta_{ab} \delta_{cd} \delta_{ef} + \frac{2^2}{n} (d_{abg} d_{gcd} \delta_{ef} + \delta_{ab} d_{cdg} d_{gef}) + \\ &+ \frac{2^2}{n} d_{abc} d_{def} + 2d_{abg} d_{gch} d_{hdv} d_{vef}. \end{aligned}$$

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